FILTERED MASS DENSITY FUNCTION FOR SUBGRID SCALE MODELING OF TURBULENT DIFFUSION FLAMES

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SUMMARY/OVERVIEW:

The objectives of this work are: (i) to further develop and improve the ``filtered density function" (FDF) methodology for modeling of the subgrid scales (SGS) in turbulent reacting flows, and (ii) to implement the resulting SGS closure for reliable large eddy simulation (LES) of turbulent diffusion flames.

TECHNICAL DISCUSSION

The filtered density function (FDF) methodology[1] has proven very effective for large eddy simulation (LES) of turbulent reacting flows.[2-6] In all contributions to-date, the FDF of the ``scalar" quantities is considered: Colucci *et al.*[2] developed a transport equation for the FDF in constant density turbulent reacting flows. Jaberi *et al.*[3] extended the methodology for LES of variable density flows by consideration of the ``filtered mass density function" (FMDF), which is essentially the mass weighted FDF. The fundamental property of the PDF methods is exhibited by the closed form nature of the chemical source term appearing in the transport equation governing the FDF (FMDF). This property is very important as evidenced in several applications of FDF for LES of a variety of turbulent reacting flows.[2-5] However, since the FDF of only the scalar quantities are considered, all of the ``hydrodynamic" effects are modeled. In all of previous simulations, these effects have been modeled via ``non-FDF" methods.

Within the past year, our efforts have been concentrated on three issues: (1) development of the FDF for SGS modeling of the velocity field, (2) development of the joint velocity-scalar FDF methodology, (3) implementation of the currently available FMDF for LES of a turbulent jet flame.

In efforts pertaining to (1), a methodology termed the velocity filtered density function (VFDF) is developed. The VFDF is basically the PDF of the SGS velocity vector. The exact transport equation governing the evolution of the VFDF is derived. It is shown that the effects of SGS convection in this equation appear in a closed form. The unclosed terms are modeled similar to that in PDF methods in Reynolds averaged simulation (RAS) procedures.[7] In this way, the

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VFDF is at least equivalent to a second-order moment SGS closure. The modeled VFDF transport equation is solved numerically via a Lagrangian Monte Carlo scheme in which the solutions of the equivalent stochastic differential equations (SDEs) are obtained. The numerical scheme preserve the Itô-Gikhman nature of the SDEs and provide a reliable solution for the VFDF. The consistency of the VFDF formulation and the convergence of its Monte Carlo solutions are assessed. This is done via comparisons between the results obtained by the Monte Carlo procedure and the finite difference solution of the transport equations of the first two filtered moments of VFDF into the LES-FD. With inclusion of the third moments from the VFDF into the LES-FD, the consistency and convergence of the Monte Carlo solution is demonstrated by good agreements of the first two SGS moments of VFDF with those obtained by LES-FD.

The VFDF predictions are compared with those with LES results with no SGS model, with the Smagorinsky[8] SGS closure, and with the dynamic Smagorinsky[9, 10] model. All of these results are also compared with direct numerical simulation (DNS) results of a three-dimensional, temporally developing mixing layer in a context similar to that conducted by Vreman *et al.*[11] This comparison provides a means of examining some of the trends and overall characteristics as predicted by LES. It is shown that the VFDF performs well in predicting some of the phenomena pertaining to the SGS transport. The magnitude of the SGS Reynolds stresses as predicted by VFDF is significantly larger than those predicted by the other SGS models and much closer to the filtered DNS results. The temporal evolution of the production rate of the SGS kinetic energy is predicted well by VFDF as compared with those via the other closures. The VFDF is also capable of accounting for the SGS backscatter without any numerical instability problems, although the level predicted is substantially less than that observed in DNS.

The results of *a priori* assessments against DNS data indicates that the values of the model coefficients as employed in VFDF are of the range suggested in the equivalent models previously used in RAS. The results of *a posteriori* assessments do not give any compelling reasons to use values other than those suggested in RAS. Most of the overall flow features, including the mean velocity field and the resolved and total Reynolds stresses as predicted by VFDF are similar to those obtained via the dynamic model. This is interesting in view of the fact that the model coefficients in VFDF are kept fixed. It may be possible to improve the predictive capabilities of the VFDF by development of a dynamic procedure to determine the model coefficients, and/or implementation of higher order closures for the generalized Langevin model parameters.[12]

In efforts pertaining to (2), a methodology termed the ``velocity-scalar filtered density function" (VSFDF) is developed. Compared to standard LES, this approach has the advantage of treating chemical reaction in a closed form; and, compared to scalar FDF has the advantage of treating convective transport (of momentum and species) in closed form. These modeling advantages have an associated computational penalty. An exact transport equation is derived for the VSFDF in which the effects of the SGS convection and chemical reaction appear in closed form. The unclosed terms in this transport equation are modeled. Again, a system of stochastic differential equations which yields statistically equivalent results to the modeled VSFDF transport equation is constructed. These SDEs are solved numerically by a Lagrangian Monte Carlo procedure in which the Itô character of the SDEs is preserved. The consistency of the proposed SDEs and the convergence of the Monte Carlo solution are currently being assessed. The VSFDF results are also being compared with those obtained via existing SGS

closures. It is expected that VSFDF will not be much more expensive than the scalar FDF, at least for multi-species turbulent flame simulations.

In efforts pertaining to (3), the FMDF methodology is being utilized for LES of a hydrocarbon jet flame. The flow field under investigation is that of a round jet in which the fuel is issued from a high-speed jet into a low speed or stagnant coflowing stream of oxidizer. This flow is inherently time-dependent and 3D. Nevertheless, some 2D (planar) simulations are also conducted (via both LES and DNS) for validation of the numerical methods and for determining the range of parameters. We have primarily considered methane/air combustion because of the rich extent of literature on methane oxidation mechanism, and availability of significant data in such flames. Up to now, we have conducted several DNS and LES of 2D and 3D jet flames. Most of the LES are conducted via the scalar FMDF methodology; the use of the joint velocity-scalar FMDF is the subject of our ongoing investigation. The SGS mixing term in this equation is modeled via the IEM closure as discussed in Ref.[3] The finite-rate chemistry effects are explicitly included in this way since the chemistry is closed in the formulation. Numerical solution of the scalar FMDF is obtained with a hybrid Eulerian/Lagrangian scheme. The hydrodynamic field is obtained by solving the filtered continuity and momentum equations with a compact parameter finite-difference scheme. The scalar quantities include mass fraction of chemical species and enthalpy. The FMDF is represented by an ensemble of Lagrangian Monte Carlo particles, which are transported in the physical space by the combined actions of large scale convection and diffusion (molecular and subgrid). Transport in the composition space occurs due to chemical reaction and SGS mixing. Thus, the grid-free Lagrangian procedure considers notional particles whose evolution can be computed stochastically to simulate motion in physical space by convection and diffusion. The compositional values of particles are changed due to mixing and reaction. The oxidation of methane is simulated via a one-step global mechanism.[13] The simulated results are used to analyze the ``spatial" and the ``compositional" structure of the flame. It is shown that the LES/FMDF predictions compare favorably with DNS data provided that the mixing frequency coefficient in the IEM closure is assigned properly. This coefficient is somewhat dependent on the flow conditions. The reason for this dependency is that the flow is not fully turbulent, specially near the inlet. Nevertheless, the values of the SGS scalar dissipation predicted by the model correlates very well with those obtained via DNS. In addition to DNS and LES/FMDF, we also simulated the jet flames via a conventional LES in which the SGS scalar correlations are ignored (this is labeled as LES-FD). A comparison between DNS and LES-FD indicates that the SGS scalar correlations have a strong influence on the large scale flow quantities; so if they are neglected the results would be erroneous.

WORK IN PROGRESS

Work is in progress on the following issues:

(I) We are considering the reduced kinetics mechanism of methane-air oxidation[13] in conjunction with the ISAT routine[15] in our scalar LES/FMDF. If this scheme proves to be computationally feasible, we will utilize it in our future simulations.

(II) We are conducting a feasibility assessment of a new computational methodology, termed the ``Spectral/hp Element" method.[16] The advantage of this methodology is that it contains spectral accuracy and it also allows for utilization of ``unstructured" grids. This assessment is being done for possible replacement of our current mean

flow solver with this methodology, so that we can consider a larger computational domain for our LES and DNS of jet flames.

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